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Authors: I. Stanković, A. Triantafyllidis, E. Mastorakos, C. Lacor and B. Merci

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ANALYSIS OF AUTO-IGNITION OF TURBULENT HYDROGEN JETS WITH DIFFERENT DETAILED REACTION MECHANISMS

I. Stanković[1*], A. Triantafyllidis[2], E. Mastorakos[2], C. Lacor[3], B. Merci[1]
[1] *Ghent University, Belgium;* [2] *Cambridge University, UK;* [3] *Vrij Universiteit Brussel, Belgium*
Ivana.Stankovic@UGent.be

Auto-ignition in turbulent non-premixed flows has significant practical applications and quite subtle fundamental aspects [1]. In numerical studies of auto-ignition phenomena, turbulence and unsteady chemistry must be modelled accurately. In order to obtain accurate simulation results for the turbulence, the Large-Eddy Simulation (LES) approach has recently received attention, while for the turbulence-chemistry interaction, the Conditional Moment Closure (CMC) can be used.

Large-Eddy Simulation (LES) results with first-order Conditional Moment Closure (CMC) are presented for a hydrogen jet, diluted with nitrogen, issuing into a turbulent co-flowing hot air stream [2]. Focus is on assessing the impact of different detailed chemical mechanisms on the auto-ignition predictions. At relatively low temperatures, where there is more uncertainty in the reaction rate constants, the choice of the detailed chemical mechanism can be of great importance. Crucial are intermediates and slow reactions, which increase the pool of reactants. Therefore, we investigate the low temperature non-premixed auto-ignition behavior with different chemical mechanisms: Li et al. [3], Mueller et al. [4] and Yetter et al. [5].

The fuel mixes with the air co-flow, ignites, and forms a lifted-like flame. The evolution of HO_2 and OH from inert to burning conditions in mixture fraction space is discussed (Figure 1). Auto-ignition of hydrogen is characterized by destruction of the pre-ignition species (HO_2) and rapid generation of OH [1]. Consistently, just upstream of the auto-ignition point (i.e. at the flame base), there is a build-up of HO_2 radical. Build-up of HO_2 ahead of the flame edge, prior to creation of H and OH, shows that base of the flame is stabilized by auto-ignition. Therefore HO_2 is a key intermediate species. The other species have low concentration at the ignition point.

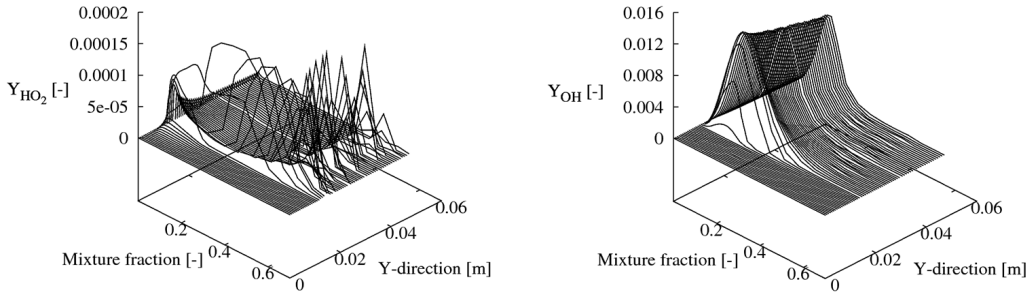

Figure 1: Evolution in the axial direction of time averaged conditional HO_2 and OH mass fractions as a function of mixture fraction (mechanism of [3]).

The trends in the experimental observations are in general well reproduced: the auto-ignition length decreases with an increase in co-flow temperature and increases with increase in co-flow velocity. With increasing co-flow temperature, the differences between the mechanisms considered diminish. In the statistically steady-state condition of the flow, reaction is balanced by convection at the flame base, showing that auto-ignition is the stabilization mechanism, with scalar dissipation rate and diffusion in physical space being relatively unimportant there.

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